through the use of reduced unit cell parameters; (2) use of a commercially available database management system, in this embodiment, Microsoft ACCESS 97, for producing the relevant crystallographic and elemental parameters and storing these and other phase data in a relational database with database "objects" such as "tables," "queries," "macros," "reports," and "modules" (Visual Basic for Applications code in this embodiment). (3) Use of experimental error limits for d_1, d_2, and ϕ to greatly reduce the number of potential solutions to examine manually in the table, (4) below, and (4) production of an output table and report which can be further customized, sorted, filtered, exported (in common formats), or further reported with common database tools, and (5) ability to customize the search to include other specific information particular to each search problem with common database tools, for example, in this embodiment Microsoft ACCESS 97.

The practice of the invention is accomplished as follows:

1. (a) The values of d_1, d_2, and ϕ, along with (b) their error limits as a constant percentage of each d-spacing (d_1, d_2) and in degrees for ϕ, and, (c) the element symbols (above atomic number 10 only) for the elements present in the sample (a maximumm of ten), are input to a computer program, ZONES, incorporating a relational database of "known materials," described herein below. A known material in the present embodiment of this invention described here is an inorganic phase present the National Institute of Standards and Technology Crystal Data file, Version J, 1997, (hereinafter referred to as NIST Crystal Data, or NIST CD, or CD—see References 2, 3, 4).

2. The computer program ZONES produces an output table of "candidate materials," defined as "known materials" which match the input requirements of 1.(a) through 1.(c), above. The output table consists of, in one line (or record) per candidate material:

(i) a unique index code (hereinafter called the "CODE") with which other information, not in the output, may be obtained from another database or other source,

(ii) a chemical formula (hereinafter called "FORMULA"),

(iii) a matching database value of d_1 in Angstroms,

(iv) a matching database value of d_2 in Angstroms,

(v) a matching database value of ϕ in degrees,

3. The "computer program incorporating a relational database of known materials" in 1., above, consists of a collection of relational database "objects," which are: (a) program "modules," in this embodiment written in Microsoft Visual Basic for Applications (VBA) computer program code, and, (b) "tables" and, (c) "queries" of the tables and other tables produced by the queries, (d) "macros" (combinations of database commands, involving tables, queries, modules, and other macros) and, (e) "reports, where "objects," "modules," "tables," "queries," "macros," and "reports" all have the common meanings usually associated with a "relational database," which is in this embodiment of the invention Microsoft ACCESS 97.

4. The CODE in 2. (i) is an index used to retrieve other information on candidate materials, for example through additional relational database tables, queries, macros, and reports.

5. The present embodiment of the "database of known materials" in 1., above, contains: (a) the following tables, wherein each table contains one or more records for each "known material," with a "record" being one line of the table (the usual definition associated with a relational database table):

(i) Database Table tblIZones2. CODE, and $100*d_1$ in Angstroms, as an integer, hereinafter referred to as "100D1; " $100*d_2$, in Angstroms, as an integer, hereinafter referred to as "100D2;" and $10*\phi$, in degrees, as an integer, hereinafter referred to as "10PHI,"

(ii) Database Table tblIFormulas. CODE and FORMULA,

(iii) Database Table tblIElements. CODE, N(1), N(2), N(3), N(4), N(5), N(6), N(7) where N(1) to N(7) are the sums of numeric element identifiers for elements with atomic numbers 1–15, 16–30, 31–45, 46–60, 61–75, 76–90, 91–105, respectively, and each numeric element identifier is 2 raised to the power: Z–15* (i–1), where, i is the index of the sums of numeric element identifiers, N(i), ranging from i=1 to i=7 (above), and Z is the atomic number of each element present, and (b) a macro, macZones, which controls the entire search/match procedure, from input to output, and which contains the following separate steps:

(i) Open Module modInputE2

(ii) Run Code E2( )

(iii) Close Module modInputE2
Element symbols are input
Values of N(i) are calculated according to 5.a (iii).

(iv) Open Query qryELE2

(v) Close Query qryELE2
Table tblIElements is queried for matching values of N(1)–N(7).
A table, tblELE, of CODE and matching N(1)–N(7) values is produced.

(vi) Open Module modERRORS

(vii) Run Code ERRDFile ( )
% errors in (d_1 and d_2), are input and written to a file.

(viii) Run Code ERRPHIFile ( )
Error in ϕ (in degrees) is input and written to a file.

(ix) Close Module modERRORS

(x) Open Query qryZones2

(xi) Close Query qryZones2
Tables tblELE, tblIZones2, and tblIFormulas are queried for materials with matching elements, and values of d_1, d_2, and ϕ within input error limits.
An output table of candidate materials, tblZones2, is produced, consisting of CODE, FORMULA, d_1, d_2, ϕ, for each.

(xii) Open Report rptzones
A Report is produced from Table tblZones2.

(xiii) Delete tblELE
Table tblELE is deleted in preparation for the next search.

The 25 zones (per each CODE or known material) of FIG. **1** are reduced in number by symmetry, with redundant combinations of d_1, d_2, ϕ, removed before storing the results in a data file as integers 100D1, 100D2, 10PHI in 5. (a) (i), above. This process is repeated for each known material with a reduced unit cell. The resulting datafile of $\leqq$25 unique combinations of 100D1, 100D2, 10PHI, and associated CODE for each known material, is read into the database as Table tblIZones2.

The database table tblIFormulas in 5. (a) (ii) is produced by reading an external datafile containing records of CODE and FORMULA for each known material into the table.

The database table tblIElements in 5. (a) (iii) is produced by reading a datafile of CODE, N(1), N(2), N(3), N(4), N(5), N(6), N(7) for each known material into the database table. This datafile is produced from the external file in 6. by searching each FORMULA for each of the 105 chemical